



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 25, 2018 – 02:50 PM EST

PDB ID : 1Q5I  
Title : Crystal structure of bacteriorhodopsin mutant P186A crystallized from bicelles  
Authors : Yohannan, S.; Faham, S.; Yang, D.; Whitelegge, J.P.; Bowie, J.U.  
Deposited on : 2003-08-07  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

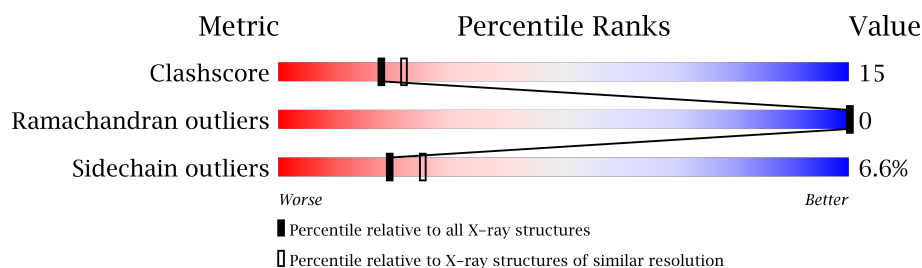
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	249	
1	B	249	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3632 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

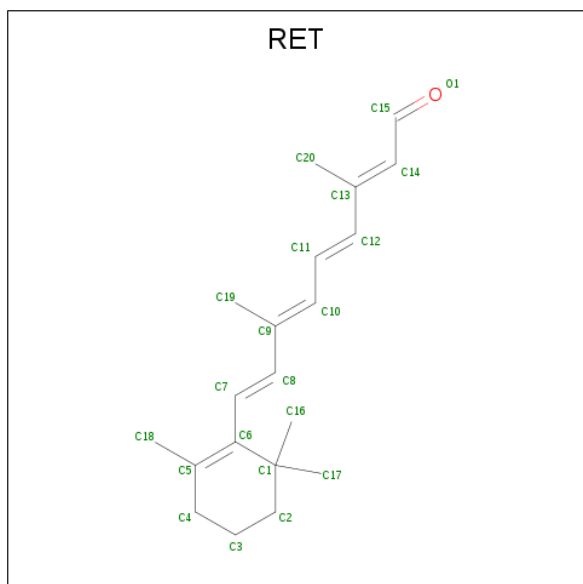
- Molecule 1 is a protein called Bacteriorhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1754	1178	268	299	9			
1	B	227	Total	C	N	O	S	0	0	0
			1754	1178	268	299	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	ALA	PRO	ENGINEERED	UNP P02945
B	186	ALA	PRO	ENGINEERED	UNP P02945

- Molecule 2 is RETINAL (three-letter code: RET) (formula: C<sub>20</sub>H<sub>28</sub>O).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			20	20		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C 20 20	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	37	Total O 37 37	0	0
3	B	47	Total O 47 47	0	0



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.63 Å   108.72 Å   56.09 Å 90.00°   113.46°   90.00°	Depositor
Resolution (Å)	500.00 – 2.30	Depositor
% Data completeness (in resolution range)	93.8 (500.00-2.30)	Depositor
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.194 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3632	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RET

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.41	0/1801	0.59	0/2459
1	B	0.41	0/1801	0.59	0/2459
All	All	0.41	0/3602	0.59	0/4918

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1754	0	1811	58	0
1	B	1754	0	1811	56	0
2	A	20	0	27	4	0
2	B	20	0	27	4	0
3	A	37	0	0	9	0
3	B	47	0	0	5	0
All	All	3632	0	3676	109	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (109) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:GLY:HA3	1:B:81:ALA:HB2	1.56	0.87
1:A:34:VAL:O	1:A:40:LYS:HE3	1.74	0.87
1:A:65:GLY:HA3	1:A:81:ALA:HB2	1.57	0.86
1:B:34:VAL:O	1:B:40:LYS:HE3	1.75	0.85
1:B:102:ASP:HB2	3:B:340:HOH:O	1.75	0.85
1:A:129:LYS:HG2	3:A:321:HOH:O	1.77	0.84
1:A:175:ARG:HH21	1:A:176:ASN:HD21	1.28	0.80
1:B:175:ARG:HH21	1:B:176:ASN:HD21	1.28	0.80
1:A:27:PHE:HA	3:A:323:HOH:O	1.82	0.80
1:A:221:LEU:O	1:A:225:ARG:HG2	1.83	0.79
1:B:221:LEU:O	1:B:225:ARG:HG2	1.84	0.79
1:B:165:PRO:HG2	3:B:345:HOH:O	1.82	0.78
1:B:169:SER:O	1:B:172:LYS:HG2	1.87	0.75
1:A:169:SER:O	1:A:172:LYS:HG2	1.89	0.73
1:B:11:ILE:HG22	3:B:336:HOH:O	1.92	0.70
1:A:136:VAL:HG12	3:A:333:HOH:O	1.96	0.66
1:B:53:ALA:HB2	1:B:216:LYS:HE2	1.77	0.65
1:B:157:THR:HA	1:B:171:PHE:HE2	1.63	0.64
1:A:64:TYR:CZ	1:B:109:LEU:HD12	2.34	0.63
1:A:157:THR:HA	1:A:171:PHE:HE2	1.63	0.62
1:B:21:GLY:HA3	3:B:334:HOH:O	2.00	0.62
1:A:53:ALA:HB2	1:A:216:LYS:HE2	1.80	0.62
1:B:9:GLU:HA	3:B:336:HOH:O	2.00	0.60
1:A:30:LYS:HB3	3:A:323:HOH:O	2.01	0.59
1:A:43:TYR:HE1	3:A:323:HOH:O	1.86	0.59
1:B:7:ARG:O	1:B:10:TRP:HD1	1.87	0.57
1:B:7:ARG:HB3	1:B:7:ARG:HH11	1.68	0.57
1:A:25:LEU:O	1:A:29:VAL:HG23	2.05	0.56
1:A:7:ARG:O	1:A:10:TRP:HD1	1.88	0.56
1:B:217:VAL:O	1:B:221:LEU:HG	2.05	0.56
1:A:7:ARG:HH11	1:A:7:ARG:HB3	1.69	0.56
1:A:8:PRO:HG2	3:A:322:HOH:O	2.06	0.56
1:B:25:LEU:O	1:B:29:VAL:HG23	2.06	0.55
1:A:51:ALA:O	1:A:55:THR:HG23	2.06	0.55
1:B:51:ALA:O	1:B:55:THR:HG23	2.07	0.54
1:A:217:VAL:O	1:A:221:LEU:HG	2.08	0.53
1:A:64:TYR:CZ	1:B:105:GLN:HG2	2.45	0.52
1:B:107:THR:HG21	1:B:156:PHE:HE1	1.74	0.52
1:A:101:VAL:HG12	1:A:160:ALA:HB2	1.91	0.52
1:A:101:VAL:CG1	1:A:160:ALA:HB2	2.40	0.52
1:A:107:THR:HG21	1:A:156:PHE:HE1	1.75	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:PHE:HE1	1:B:221:LEU:HD23	1.75	0.52
1:B:101:VAL:HG12	1:B:160:ALA:HB2	1.91	0.51
1:A:64:TYR:OH	1:B:105:GLN:HG2	2.11	0.51
1:B:101:VAL:CG1	1:B:160:ALA:HB2	2.41	0.50
1:A:140:ILE:HD12	3:A:333:HOH:O	2.12	0.50
1:A:69:VAL:HG13	3:A:321:HOH:O	2.11	0.49
1:B:181:LEU:HD13	1:B:215:ALA:HB2	1.94	0.49
1:A:27:PHE:HE1	1:A:221:LEU:HD23	1.77	0.49
1:A:169:SER:O	1:A:172:LYS:HE2	2.13	0.49
1:A:181:LEU:HD13	1:A:215:ALA:HB2	1.95	0.48
1:B:53:ALA:HA	1:B:85:ASP:OD2	2.13	0.48
1:B:186:ALA:HB2	2:B:301:RET:H183	1.95	0.48
1:A:53:ALA:HA	1:A:85:ASP:OD2	2.13	0.48
1:B:107:THR:CG2	1:B:156:PHE:HE1	2.27	0.48
1:B:189:TRP:CD1	2:B:301:RET:H22	2.48	0.48
1:A:98:ALA:HB1	1:A:103:ALA:HB3	1.96	0.48
1:B:157:THR:HA	1:B:171:PHE:CE2	2.46	0.48
1:A:189:TRP:CD1	2:A:301:RET:H22	2.48	0.48
1:B:169:SER:O	1:B:172:LYS:HE2	2.14	0.48
1:B:7:ARG:O	1:B:10:TRP:CD1	2.67	0.48
1:B:13:LEU:HD13	1:B:205:THR:HG21	1.96	0.47
1:A:157:THR:HA	1:A:171:PHE:CE2	2.47	0.47
1:A:16:GLY:O	1:A:20:MET:HG2	2.14	0.46
1:B:86:TRP:CD1	2:B:301:RET:H14	2.50	0.46
1:A:107:THR:CG2	1:A:156:PHE:HE1	2.28	0.46
1:B:83:TYR:CD2	1:B:123:LEU:HD13	2.50	0.46
1:B:98:ALA:HA	1:B:156:PHE:CE2	2.51	0.46
1:A:172:LYS:CG	1:A:173:VAL:N	2.79	0.46
1:A:98:ALA:HA	1:A:156:PHE:CE2	2.51	0.46
1:A:32:MET:O	1:B:129:LYS:HE3	2.17	0.45
1:A:209:MET:HG3	1:A:210:VAL:N	2.30	0.45
1:B:209:MET:HG3	1:B:210:VAL:N	2.31	0.45
1:A:83:TYR:CD2	1:A:123:LEU:HD13	2.50	0.45
1:B:98:ALA:HB1	1:B:103:ALA:HB3	1.99	0.45
1:A:184:ALA:O	1:A:188:VAL:HG23	2.17	0.45
1:A:86:TRP:CD1	2:A:301:RET:H14	2.52	0.45
1:A:141:SER:OG	2:A:301:RET:H41	2.16	0.45
1:B:184:ALA:O	1:B:188:VAL:HG23	2.17	0.45
1:A:64:TYR:CE1	1:B:105:GLN:HG2	2.52	0.44
1:B:172:LYS:CG	1:B:173:VAL:N	2.80	0.44
1:B:16:GLY:O	1:B:20:MET:HG2	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ARG:HH21	1:A:176:ASN:ND2	2.05	0.44
1:A:186:ALA:HB2	2:A:301:RET:H183	1.99	0.44
1:B:71:PHE:CE2	1:B:134:ARG:CZ	3.01	0.44
1:B:175:ARG:HH21	1:B:176:ASN:ND2	2.05	0.44
1:A:172:LYS:HG3	1:A:173:VAL:N	2.32	0.44
1:A:156:PHE:HB3	1:A:171:PHE:CZ	2.53	0.44
1:A:36:ASP:HA	1:A:37:PRO:HD3	1.89	0.44
1:A:13:LEU:HD13	1:A:205:THR:HG21	2.00	0.43
1:B:36:ASP:HA	1:B:37:PRO:HD3	1.89	0.43
1:B:28:LEU:HD22	1:B:28:LEU:O	2.18	0.43
1:B:172:LYS:HG3	1:B:173:VAL:N	2.33	0.43
1:B:15:LEU:O	1:B:19:LEU:HG	2.18	0.43
1:A:15:LEU:O	1:A:19:LEU:HG	2.18	0.42
1:B:141:SER:OG	2:B:301:RET:H41	2.19	0.42
1:A:7:ARG:O	1:A:10:TRP:CD1	2.68	0.42
1:B:206:LEU:O	1:B:210:VAL:HG23	2.18	0.42
1:B:30:LYS:HE2	1:B:43:TYR:OH	2.20	0.42
1:A:206:LEU:O	1:A:210:VAL:HG23	2.19	0.41
1:A:90:THR:N	1:A:91:PRO:HD2	2.35	0.41
1:A:49:VAL:CG1	1:A:216:LYS:HG2	2.49	0.41
1:B:156:PHE:HB3	1:B:171:PHE:CZ	2.56	0.41
1:A:169:SER:HA	1:A:172:LYS:HD3	2.01	0.41
1:A:70:PRO:HD2	3:A:321:HOH:O	2.21	0.41
1:B:49:VAL:CG1	1:B:216:LYS:HG2	2.50	0.41
1:A:30:LYS:HE2	1:A:43:TYR:OH	2.21	0.41
1:B:7:ARG:HA	1:B:8:PRO:HD3	1.94	0.41
1:B:90:THR:N	1:B:91:PRO:HD2	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	225/249 (90%)	222 (99%)	3 (1%)	0	100	100
1	B	225/249 (90%)	222 (99%)	3 (1%)	0	100	100
All	All	450/498 (90%)	444 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	181/194 (93%)	169 (93%)	12 (7%)	19	25
1	B	181/194 (93%)	169 (93%)	12 (7%)	19	25
All	All	362/388 (93%)	338 (93%)	24 (7%)	19	25

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	13	LEU
1	A	15	LEU
1	A	28	LEU
1	A	38	ASP
1	A	58	LEU
1	A	94	LEU
1	A	109	LEU
1	A	131	TYR
1	A	152	LEU
1	A	209	MET
1	A	227	ARG
1	B	7	ARG
1	B	13	LEU
1	B	15	LEU
1	B	28	LEU
1	B	38	ASP
1	B	58	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	94	LEU
1	B	109	LEU
1	B	131	TYR
1	B	152	LEU
1	B	209	MET
1	B	227	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	ASN
1	B	176	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	RET	A	301	1	19,20,21	2.02	4 (21%)	27,27,28	2.64	11 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	RET	B	301	1	19,20,21	2.01	4 (21%)	27,27,28	2.62	11 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	RET	A	301	1	-	0/13/30/31	0/1/1/1
2	RET	B	301	1	-	0/13/30/31	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	RET	C17-C1	2.37	1.58	1.53
2	B	301	RET	C4-C5	2.41	1.56	1.51
2	B	301	RET	C17-C1	2.68	1.59	1.53
2	A	301	RET	C4-C5	2.74	1.56	1.51
2	B	301	RET	C5-C6	4.25	1.41	1.34
2	A	301	RET	C5-C6	4.38	1.42	1.34
2	A	301	RET	C1-C6	5.40	1.61	1.53
2	B	301	RET	C1-C6	5.45	1.61	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	RET	C8-C9-C10	-4.82	111.55	118.94
2	A	301	RET	C8-C9-C10	-4.68	111.77	118.94
2	A	301	RET	C11-C10-C9	-4.11	121.44	127.31
2	B	301	RET	C11-C10-C9	-4.06	121.51	127.31
2	A	301	RET	C10-C11-C12	-3.85	111.42	123.23
2	B	301	RET	C10-C11-C12	-3.74	111.77	123.23
2	B	301	RET	C7-C6-C5	-3.22	113.85	121.54
2	A	301	RET	C7-C6-C5	-3.22	113.85	121.54
2	A	301	RET	C12-C13-C14	-3.03	109.05	118.83
2	B	301	RET	C12-C13-C14	-3.03	109.07	118.83
2	A	301	RET	C18-C5-C4	-2.70	108.33	113.45
2	B	301	RET	C18-C5-C4	-2.68	108.38	113.45
2	B	301	RET	C2-C1-C6	2.74	114.76	110.48
2	B	301	RET	C19-C9-C8	2.94	122.78	118.10
2	A	301	RET	C2-C1-C6	2.94	115.08	110.48
2	A	301	RET	C19-C9-C8	2.94	122.79	118.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	RET	C1-C6-C7	3.10	124.44	115.73
2	B	301	RET	C1-C6-C7	3.10	124.45	115.73
2	A	301	RET	C20-C13-C12	3.43	123.57	118.10
2	B	301	RET	C20-C13-C12	3.58	123.80	118.10
2	B	301	RET	C18-C5-C6	6.24	131.49	124.51
2	A	301	RET	C18-C5-C6	6.44	131.71	124.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	RET	4	0
2	B	301	RET	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.